CHARACTERIZATION OF MICROSOLVATED 15C5 CROWN ETHER FROM BROADBAND ROTATIONAL SPECTROSCOPY

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15-crown-5 ether (15C5) and its complexes with water generated in a supersonic jet have been studied using broadband Fourier transform microwave spectroscopy. The most stable form of the crown ether not previously reported, to complete a total of nine isolated forms, has been detected. In addition, two 1:1 and two 1:2 clusters have been observed. The clusters structures have been unambiguously identified through the observation of water ^{18}O isotopologue spectra and a detailed analysis of the rotational parameters. The structures of all the clusters show that at least one water molecule, located close to the axis of the ring, interacts through two simultaneous hydrogen bonds to the endocyclic oxygen atoms. This interaction reshapes the 15C5 ring to reduce its rich conformational panorama to only two open structures, related to those found in complexes with Li^+ or Na^+ ions. In the most intense 1:2 form, the two water molecules repeat the same interaction scheme in both sides of the ring while in the second one the water molecules lie on the same side of the ring.